Journal of Applied Physics 2013 vol.113 N11

Impact of isovalent doping on the trapping of vacancy and interstitial related defects in Si

Sgourou E., Timerkaeva D., Londos C., Aliprantis D., Chroneos A., Caliste D., Pochet P.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

We investigate the impact of isovalent (in particular lead (Pb)) doping on the production and thermal stability of the vacancy-related (VO) and the interstitial-related (CiOi and CiCs) pairs in 2 MeV electron irradiated Si samples. We compare the Cz-Si samples with high and low carbon concentration, as well as with Pb-C and Ge-C codoped samples. Using Fourier Transform Infrared Spectroscopy (FTIR), we first determine that under the examined conditions the production of VO decreases with the increase of the covalent radius of the prevalent dopant. Moreover, the production of the VO, CiOi, and CiCs pairs is quite suppressed in Pb-doped Si. In addition, we conclude to an enhanced trapping of both Ci and Cs by Pb impurity under irradiation. The results are further discussed in view of density functional theory calculations. The relative thermodynamic stability of carbon and interstitial related complexes was estimated through the calculations of binding energies of possible defect pairs. This allows to investigate the preferred trapping of vacancies in Pb-doped samples and interstitials in the Ge-doped samples. The different behavior is revealed by considering the analysis of the ratio of vacancy-related to interstitial-related clusters derived from the FTIR measurements. The presence of PbV complexes is confirmed due to the mentioned analysis. © 2013 American Institute of Physics.

http://dx.doi.org/10.1063/1.4795510